

Screening effects on the excitonic instability in graphene

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We investigate the excitonic instability in the theory of Dirac fermions in graphene with long-range Coulomb interaction. We analyze the electron-hole vertex relevant for exciton condensation in the ladder approximation, showing that it blows up at a critical value of the interaction strength $\alpha = e^2/4\pi v_F$ sensitive to further many-body corrections. Under static screening of the interaction, we find that taking into account electron self-energy corrections increases the critical coupling to $\alpha_c \approx 2.09$, for a number $N = 4$ of two-component Dirac fermions. We show that the dynamical screening of the interaction has however the opposite effect of enhancing the instability, which turns out to develop then at $\alpha_c \approx 0.99$ for $N = 4$, bringing the question of whether that critical value can be reached by the effective coupling in real graphene samples at the low-energy scales of the exciton condensation.

Introduction.— The discovery of graphene, the material made of a one-atom-thick carbon layer, has attracted a lot attention as it provides the realization of a system where the electrons have conical valence and conduction bands, therefore behaving at low energies as massless Dirac fermions[1–3]. This offers the possibility of employing the new material as a test ground of fundamental concepts in theoretical physics, since the interacting electron system represents a variant of strongly coupled quantum electrodynamics (QED) affording quite unusual effects[4–7].

A remarkable feature of such a theory is that a sufficiently strong Coulomb interaction may open a gap in the electronic spectrum. This effect, already known from the study of QED [8], was first addressed in graphene in the context of the theory with a large number N of fermion flavors[9–12]. The existence of a critical point for exciton condensation was also suggested from second-order calculations of electron self-energy corrections[13]. More recently, Monte Carlo simulations of the field theory have been carried out on the graphene lattice[14, 15], showing that the chiral symmetry of the massless theory can be broken at the physical value $N = 4$ above a critical interaction strength $\alpha_c \approx 1.08$ [14]. The possibility of exciton condensation has been also studied in the ladder approximation[16–19], leading in the case of static screening of the interaction to an estimate of the critical coupling $\alpha_c \approx 1.62$ for $N = 4$ [16]. Lately, the resolution of the Schwinger-Dyson formulation of the gap equation has revealed that the effect of the dynamical polarization can significantly lower the critical coupling for exciton condensation, down to a value $\alpha_c \approx 0.92$ for $N = 4$ [20].

In this paper we take advantage of the renormalization properties of the Dirac theory in order to assess the effect of different many-body corrections to the excitonic instability. In this respect, the renormalization of the quasiparticle properties can have a significant impact, mainly through the increase of the Fermi velocity at low energies[21, 22]. Thus, we will consider the renormalization of the electron-hole vertex accounting for the exciton condensation in the ladder approximation, supplemented by self-energy corrections to electron and hole

states. This dressing of the bare quasiparticles will have the result of increasing the critical coupling at which the excitonic instability takes place, going in the same direction as the effect of screening the Coulomb interaction. We will see however that, incorporating the dynamical polarization in the ladder approximation, the screening effects are softened at $N = 4$, leading to values of the critical coupling below those corresponding to the nominal interaction strength in isolated free-standing graphene.

We consider the field theory for Dirac quasiparticles in graphene interacting through the long-range Coulomb potential, with a Hamiltonian given by

$$H = iv_F \int d^2r \bar{\psi}_i(\mathbf{r}) \boldsymbol{\gamma} \cdot \nabla \psi_i(\mathbf{r}) + \frac{e^2}{8\pi} \int d^2r_1 \int d^2r_2 \rho(\mathbf{r}_1) \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \rho(\mathbf{r}_2) \quad (1)$$

where $\{\psi_i\}$ is a collection of $N/2$ four-component Dirac spinors, $\bar{\psi}_i = \psi_i^\dagger \gamma_0$, and $\rho(\mathbf{r}) = \bar{\psi}_i(\mathbf{r}) \gamma_0 \psi_i(\mathbf{r})$. The matrices γ_σ satisfy $\{\gamma_\mu, \gamma_\nu\} = 2 \text{diag}(1, -1, -1)$ and can be conveniently represented in terms of Pauli matrices as $\gamma_{0,1,2} = (\sigma_3, \sigma_3 \sigma_1, \sigma_3 \sigma_2) \otimes \sigma_3$, where the first factor acts on the two sublattice components of the graphene lattice.

Our main interest is to study the behavior of the vertex for the operator $\rho_m(\mathbf{r}) = \bar{\psi}(\mathbf{r}) \psi(\mathbf{r})$. This gives the order parameter for the exciton condensation, and the signal that it gets a nonvanishing expectation value can be obtained from the divergence of $\langle T \rho_m(\mathbf{q}, t) \rho_m(-\mathbf{q}, 0) \rangle$. The singular behavior of this susceptibility can be traced back to the divergence of the vertex for $\langle \rho_m(\mathbf{q}) \psi(\mathbf{k} + \mathbf{q}) \psi^\dagger(\mathbf{k}) \rangle$ at $\mathbf{q} \rightarrow 0$. We will denote the vertex in this limit (setting also the corresponding frequency $\omega_q = 0$) by $\Gamma(\mathbf{k}, \omega_k)$. In the ladder approximation, depicted diagrammatically in Fig. 1, the vertex is bound to satisfy the equation

$$\Gamma(\mathbf{k}, \omega_k) = \gamma_0 + \int \frac{d^2p}{(2\pi)^2} \frac{d\omega_p}{2\pi} \frac{\Gamma(\mathbf{p}, \omega_p)}{v_F^2 \mathbf{p}^2 + \omega_p^2} V(\mathbf{k} - \mathbf{p}, i\omega_k - i\omega_p) \quad (2)$$

where $V(\mathbf{p}, \omega_p)$ stands for the Coulomb interaction. We will deal in general with the RPA to screen the potential, so that $V(\mathbf{p}, \omega_p) = e^2/(2|\mathbf{p}| + e^2\chi(\mathbf{p}, \omega_p))$, in terms of the polarization χ for N two-component Dirac fermions.

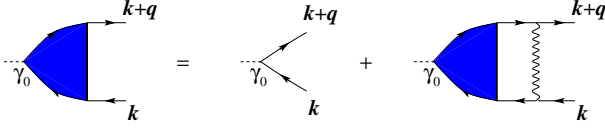


FIG. 1: Self-consistent diagrammatic equation for the vertex of $\langle \rho_m(\mathbf{q}) \psi(\mathbf{k} + \mathbf{q}) \psi^\dagger(\mathbf{k}) \rangle$, equivalent to the sum of ladder diagrams built from the iteration of the Coulomb interaction (wavy line) between electron and hole states (arrow lines).

Eq. (2) is formally invariant under a dilatation of frequencies and momenta, which shows that the scale of $\Gamma(\mathbf{k}, \omega_k)$ is dictated by the high-energy cutoff Λ needed to regularize the integrals. The vertex acquires in general an anomalous dimension γ_{ψ^2} , which governs the behavior under changes in the cutoff[23]

$$\Gamma(\mathbf{k}, \omega_k) \sim \Lambda^{\gamma_{\psi^2}} \quad (3)$$

We recall below how to compute γ_{ψ^2} , showing that it diverges at a critical value of the interaction strength. This translates into a divergence of the own susceptibility at momentum transfer $\mathbf{q} \rightarrow 0$, providing then the signature of the condensation of $\rho_m(\mathbf{r}) = \bar{\psi}(\mathbf{r})\psi(\mathbf{r})$ and the consequent development of the excitonic gap.

Self-energy corrections to ladder approximation.— We deal first with the approach in which electrons and holes are dressed by self-energy corrections, while the Coulomb interaction in (2) is screened by means of the static RPA with $\chi(\mathbf{p}, 0) = (N/16)|\mathbf{p}|/v_F$. It is known that graphene remains a conventional Fermi liquid even at the charge neutrality point, with a quasiparticle weight that does not vanish at the Fermi level[24]. The most important self-energy effect comes from the renormalization of the Fermi velocity at low energies[25], and this is the feature that we want to incorporate in our analysis, identifying v_F in Eq. (2) with the Fermi velocity dressed by self-energy corrections.

The electron self-energy corrections, as well as the terms of the ladder series, are given by logarithmically divergent integrals that need to be cut off at a given scale Λ . Alternatively, one can also define the theory at spatial dimension $d = 2 - \epsilon$, what automatically regularizes all the momentum integrals. Eq. (2) then becomes

$$\Gamma(\mathbf{k}, 0) = \gamma_0 + \frac{e_0^2}{4\kappa} \int \frac{d^d p}{(2\pi)^d} \Gamma(\mathbf{p}, 0) \frac{1}{\tilde{v}_F(\mathbf{p})|\mathbf{p}|} \frac{1}{|\mathbf{p} - \mathbf{k}|} \quad (4)$$

where $\tilde{v}_F(\mathbf{p})$ is the Fermi velocity dressed with the self-energy corrections, $\kappa = 1 + Ne^2/32v_F$, and e_0^2 is related to e^2 through an auxiliary momentum scale ρ such that $e_0^2 = \rho^\epsilon e^2$.

In the ladder approximation, the Fermi velocity gets a divergent correction only from the “rainbow” self-energy diagram with exchange of a single screened interaction[25]. The dressed Fermi velocity becomes

$$\tilde{v}_F(\mathbf{p}) = v_F + \frac{e_0^2}{\kappa} \frac{1}{(4\pi)^{2-\epsilon/2}} \frac{\Gamma(\frac{\epsilon}{2})\Gamma(\frac{1-\epsilon}{2})\Gamma(\frac{3-\epsilon}{2})}{\Gamma(2-\epsilon)} \frac{1}{|\mathbf{p}|^\epsilon} \quad (5)$$

The expressions (4) and (5) are singular in the limit $\epsilon \rightarrow 0$. The most convenient way to show that all the divergences can be renormalized away is to resort at this point to a perturbative computation of $\Gamma(\mathbf{k}, 0)$.

The solution of (4) can be obtained in the form

$$\Gamma(\mathbf{k}, 0) = \gamma_0 \left(1 + \sum_{n=1}^{\infty} \lambda_0^n \frac{r_n}{|\mathbf{k}|^{n\epsilon}} \right) \quad (6)$$

with $\lambda_0 = e_0^2/4\pi\kappa v_F$. Each term in the sum can be obtained from the previous one by noticing that

$$\begin{aligned} \int \frac{d^d p}{(2\pi)^d} \frac{1}{|\mathbf{p}|^{(m-1)\epsilon}} \frac{1}{|\mathbf{p}|} \frac{1}{|\mathbf{p} - \mathbf{k}|} \\ = \frac{(4\pi)^{\epsilon/2}}{4\pi^{3/2}} \frac{\Gamma(\frac{m\epsilon}{2})\Gamma(\frac{1-m\epsilon}{2})\Gamma(\frac{1-\epsilon}{2})}{\Gamma(\frac{1+(m-1)\epsilon}{2})\Gamma(1-\frac{m+1}{2}\epsilon)} \frac{1}{|\mathbf{k}|^{m\epsilon}} \end{aligned} \quad (7)$$

At each given perturbative level, the vertex displays then a number of poles in the variable ϵ . The crucial point is that these divergences can be reabsorbed by passing to physical quantities such that $v_F = Z_v(v_F)_{\text{ren}}$ and $\bar{\psi}\psi = Z_{\psi^2}(\bar{\psi}\psi)_{\text{ren}}$ (the scale of the single Dirac field is not renormalized in the ladder approximation).

The renormalized vertex $\Gamma_{\text{ren}} = Z_{\psi^2}\Gamma$ can be actually made finite with a suitable choice of momentum-independent factors Z_v and Z_{ψ^2} . Z_v must be chosen to cancel the $1/\epsilon$ pole in (5), and it has therefore the simple structure $Z_v = 1 + b_1/\epsilon$, with $b_1 = -e^2/16\pi\kappa(v_F)_{\text{ren}}$. On the other hand, we have the general structure

$$Z_{\psi^2} = 1 + \sum_{n=1}^{\infty} \frac{c_n}{\epsilon^n} \quad (8)$$

The position of the different poles must be chosen to enforce the finiteness of $\Gamma_{\text{ren}} = Z_{\psi^2}\Gamma$ in the limit $\epsilon \rightarrow 0$. The computation of the first orders of the expansion gives for instance the result

$$\begin{aligned} c_1(\lambda) &= -\frac{1}{2}\lambda - \frac{1}{8}\log(2)\lambda^2 - \frac{1}{1152}(\pi^2 + 120\log^2(2))\lambda^3 \\ &\quad - \frac{10\pi^2\log(2)+688\log^3(2)+15\zeta(3)}{6144}\lambda^4 \\ &\quad - \frac{13\pi^4+2064\pi^2\log^2(2)+144(716\log^4(2)+37\log(2)\zeta(3))}{737280}\lambda^5 \\ &\quad + \dots \\ c_2(\lambda) &= \frac{1}{16}\lambda^2 + \frac{1}{24}\log(2)\lambda^3 + \frac{1}{18432}(5\pi^2 + 744\log^2(2))\lambda^4 \\ &\quad + \frac{110\pi^2\log(2)+8592\log^3(2)+135\zeta(3)}{184320}\lambda^5 + \dots \\ c_3(\lambda) &= -\frac{1}{768}\log(2)\lambda^4 - \frac{1}{184320}(\pi^2 + 360\log^2(2))\lambda^5 + \dots \\ c_4(\lambda) &= -\frac{1}{7680}\log(2)\lambda^5 + \dots \end{aligned} \quad (9)$$

where the series are written in terms of the renormalized coupling $\lambda \equiv \rho^{-\epsilon} Z_v \lambda_0$

The physical observable in which we are interested is the anomalous dimension γ_{ψ^2} . The change in the dimension of Γ_{ren} comes from the dependence of Z_{ψ^2} on the only dimensionful scale ρ , being $\gamma_{\psi^2} = (\rho/Z_{\psi^2})\partial Z_{\psi^2}/\partial\rho$ [23]. The bare theory at $d \neq 2$ does not know about the

arbitrary scale ρ , and the independence of $\lambda_0 = \rho^\epsilon \lambda / Z_v$ on that variable leads to

$$\rho \frac{\partial \lambda}{\partial \rho} = -\epsilon \lambda - \lambda b_1(\lambda) \quad (10)$$

The anomalous dimension is then[26]

$$\gamma_{\psi^2} = \rho \frac{\partial \lambda}{\partial \rho} \frac{\partial \log Z_{\psi^2}}{\partial \lambda} = -\lambda c'_1(\lambda) \quad (11)$$

In the derivation of (11), it has been implicitly assumed that poles in the variable ϵ cannot appear at the right-hand-side of the equation. For this to be true, the set of equations $c'_{n+1} = c_n c'_1 - b_1 c'_n$ must be satisfied identically[26]. Quite remarkably, we have verified that this is the case, up to the order λ^7 we have computed the coefficients in (8). This is the proof of the renormalizability of the theory, which guarantees that physical quantities like γ_{ψ^2} remain finite in the limit $\epsilon \rightarrow 0$.

From the practical point of view, the important result is the evidence that the perturbative expansion of $c_1(\lambda)$ approaches a geometric series in the λ variable. It can be checked that the coefficients in the expansion grow exponentially with the order n , in such a way that

$$-c_1(\lambda) \geq \sum_{n=1}^{\infty} d^n \lambda^n \quad (12)$$

A lower bound for d can be obtained from the first orders in $c_1(\lambda)$. This estimate tends to increase as it is made from higher orders in the expansion. The assumption of scaling with the order n allows us to estimate a radius of convergence $\lambda_c \approx 0.49$ (to be compared with the value in the approach neglecting self-energy corrections, which leads to $\lambda_c \approx 0.45$ [18], in close agreement with the result of Ref. 16). The critical coupling in the variable $\lambda = \alpha/\kappa$ can be used to draw the boundary for exciton condensation in the (N, α) phase diagram, represented in Fig. 2. For $N = 4$, we get in particular the critical coupling $\alpha_c \approx 2.09$, significantly above the critical value that would be obtained from the radius of convergence without self-energy corrections ($\alpha_c \approx 1.53$).

Dynamical screening in the ladder approximation.— In the framework of the ladder approximation, one can also study the effect of the dynamical screening of the Coulomb interaction. We can go beyond the static RPA by taking into account the full effect of the frequency-dependent polarization, which for Dirac fermions takes the form $\chi(\mathbf{p}, \omega_p) = (N/16) \mathbf{p}^2 / \sqrt{v_F^2 \mathbf{p}^2 - \omega_p^2}$ [25]. This expression can be introduced in Eq. (2) to look again for self-consistent solutions for the vertex $\Gamma(\mathbf{k}, \omega_k)$. While this problem does not afford an analytic approach of the type shown before, one can resort to numerical methods for the resolution of the integral equation. In this procedure, we find again that there is a critical coupling at which $\Gamma(\mathbf{k}, \omega_k)$ blows up, marking the boundary between two different regimes where the integral equation has respectively positive and negative (unphysical) solutions.

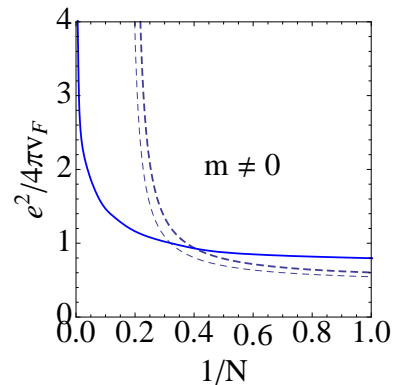


FIG. 2: Phase diagram showing the boundary of the phase with exciton condensation ($m \neq 0$), obtained in the ladder approximation with and without electron self-energy corrections (upper and lower dashed lines) and with dynamical screening of the Coulomb interaction (full line).

In practice, we have solved the integral equation (2) by defining the vertex in a discrete set of points in frequency and momentum space. One can take as independent variables in $\Gamma(\mathbf{k}, \omega_k)$ the modulus of \mathbf{k} and positive frequencies ω_k , and we have adopted accordingly a grid of dimension $l \times l$ covering those variables. The advantage of this approach is that the number l plays the role of cutoff, making straightforward to assess the effect of higher frequencies and momenta as l is increased. We have solved the integral equation in $l \times l$ grids with l running up to a value of 200, for which it is still viable to invert a matrix of dimension l^2 . One can rely moreover on the scale invariance of the theory to find the trend at larger values of l , as the critical coupling α_c must obey a well-defined finite-size scaling law as a function of the cutoff $\alpha_c(l) = \alpha_c(\infty) + c/l^\nu$.

For a given value of N , we have determined the critical point at which the vertex $\Gamma(\mathbf{k}, \omega_k)$ blows up. The value of $\alpha_c(l)$ for our largest l provides an upper bound for the critical coupling in the continuum limit, as $\alpha_c(l)$ turns out to be always a decreasing function of the variable l . On the other hand, the use of the above finite-size scaling law allows to estimate $\alpha_c(\infty)$. We have chosen to represent in Fig. 2 the conservative upper bound $\alpha_c(200)$ as a function of N . In marked difference with other approaches, we observe that now a critical coupling always exists, no matter how large the value of N may be. For $N = 4$ corresponding to graphene, we get the values $\alpha_c(200) \approx 1.08$ and $\alpha_c(\infty) \approx 0.99$.

We see that the value of the critical coupling obtained upon dynamical screening of the interaction is substantially smaller than the value found for $N = 4$ in the static approximation. This agrees with the results obtained in Ref. [20], where the resolution of the gap equation was accomplished taking into account the frequency-dependent polarization. The critical coupling obtained there for $N = 4$, $\alpha_c \approx 0.92$, is actually very close to our

estimate $\alpha_c(\infty) \approx 0.99$. These values are also close to the critical coupling $\alpha_c \approx 1.08$ found in lattice Monte Carlo simulations[14], suggesting that the consideration of the dynamical screening provides a most sensible approximation to the excitonic instability.

Conclusion.— We have shown that the various many-body corrections used to dress the electron quasiparticles and the Coulomb interaction can have significant impact on the excitonic instability. The effects of the electron self-energy corrections and the electron-hole polarization have an important role in reducing the strength of the instability. We have seen however that, as anticipated in Ref. [20], the simple static approximation overestimates the screening effects, and that a more accurate approach to the problem requires the consideration of the dynamical screening of the interaction.

It is puzzling that, if we were to use the nominal values of the parameters appropriate for graphene, we would arrive at the conclusion that an isolated free-standing layer of the material (for which $\alpha \approx 2.2$) should be in the phase of exciton condensation. This is at odds with the absence of any experimental observation of a gap in suspended graphene samples. Our many-body analysis shows that

the only possible relevant effects that have been dismissed are those related to the scaling of the quasiparticle parameters. In this respect, the growth of the Fermi velocity at low energies[24] can have a deep impact to prevent the excitonic instability[22, 27]. This effect, expressed by the scaling law (10) at $\epsilon = 0$, has been already observed in experimental samples of graphene at very low doping levels[28]. It is quite plausible that, at the low-energy scales where the gap could develop (about three orders of magnitude below the scale of the high-energy cutoff), the scaling of the Fermi velocity may have driven the effective coupling to such small values that the excitonic instability cannot then proceed. This can be one more consequence of the nontrivial scaling properties of the theory of Dirac fermions, implying that the electrons in graphene approach a noninteracting regime as they are observed at energies arbitrarily closer to the charge neutrality point.

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